Phthalic acid, 2-propylphenyl tetradecyl ester

Inchi: InChI=1S/C31H44O4/c1-3-5-6-7-8-9-10-11-12-13-14-19-25-34-30(32)27-22-16-17-23-28
InchiKey: KMVCIOKOFUFQJU-UHFFFAOYSA-N
Formula: C31H44O4
SMILES: CCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1ccccc1CCC
Mol. weight [g/mol]: 480.68

Physical Properties

Property code	Value	Unit	Source
gf	-52.14	kJ/mol	Joback Method
hf	-722.65	kJ/mol	Joback Method
hfus	68.92	kJ/mol	Joback Method
hvap	108.79	kJ/mol	Joback Method
log10ws	-10.46		Crippen Method
logp	8.716		Crippen Method
mcvol	415.010	ml/mol	McGowan Method
pc	830.50	kPa	Joback Method
rinpol	3439.00		NIST Webbook
rinpol	3439.00		NIST Webbook
tb	1124.58	K	Joback Method
tc	1383.23	K	Joback Method
tf	661.33	K	Joback Method
vc	1.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1445.92	J/mol×K	1124.58	Joback Method
cpg	1460.95	J/mol×K	1167.69	Joback Method
cpg	1474.05	J/mol×K	1210.80	Joback Method
cpg	1485.31	J/mol×K	1253.90	Joback Method
cpg	1494.87	J/mol×K	1297.01	Joback Method
cpg	1502.81	J/mol×K	1340.12	Joback Method
cpg	1509.27	J/mol×K	1383.23	Joback Method
dvisc	0.0001302	Pa×s	661.33	Joback Method

dvisc	0.0000699	Pa×s	738.54	Joback Method
dvisc	0.0000423	Pa×s	815.75	Joback Method
dvisc	0.0000279	Pa×s	892.95	Joback Method
dvisc	0.0000196	Pa×s	970.16	Joback Method
dvisc	0.0000146	Pa×s	1047.37	Joback Method
dvisc	0.0000113	Pa×s	1124.58	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357029&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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